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WHAT IS CLAIMED IS:

- 1. A process for identifying compounds as potential ligands for a protein having a ligand-binding site, comprising:
 - a) determining secondary structural elements of the protein that constitute the ligand-binding site;
 - b) breaking down the molecular surface of the ligand-biding site of the protein into molecular surface elements;
 - (c) identifying known molecular surface patches that are complementary to a neighboring molecular surface element;
 - (d) effecting coordinate transformation of the molecular surface patches identified in step c) with a neighboring molecular surface element, based on a starting element at an rms value less than 2Å;
 - (e) identifying counterparts of the molecular surface patches in known compounds; and
 - (f) assessing the fit of the compounds identified in step (e) in terms of local packing density, wherein a better fit indicates a better potential for the compounds to be ligands of the protein.
- 2. The process as described in claim 1, wherein external surfaces of the secondary structures of the ligand binding site are determined in step (b).
- 3. The process as described in claim 1 wherein the known molecular surface patches are superposed with the secondary structural elements.
- 4. The process as described in Claim 1 wherein the molecular surface patches lie on atoms of the binding site after a coordinate transformation.
- 5. The process as described in Claim 1, wherein the identified ligands are compared with a known initial protein plus ligand.
 - 6. The process as described in claim 1, wherein the ligands are peptides.
 - 7. The process as described in claim 1 wherein the proteins are enzymes.
 - 8. The process as described in claim 1, wherein the rms value is 1.5 Å.
- 9. The process of Claim 1 wherein the known molecular surface patches are identified from a database.

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- 10. The process of Claim 1 wherein the known neighboring element is a receptor or an enzyme.
- 11. The process as described in claim 6, wherein the peptides comprise at least 10 amino acids.
- 12. The process as described in claim 6 wherein the peptides are subsequently transformed into a peptidomimetic.
- 13. A process of determining the structure of a protein, comprising: identifying ligands from known molecular surface patches using the process of claim 1; and determining the structure of the protein based on the known structure of the neighboring element to which the molecular surface patches bind.
- 14. The process as described in claim 2, wherein the molecular surface patches create contact with said external surfaces.